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PII: S0093-6413(21)00030-6
DOI: https://doi.org/10.1016/j.mechrescom.2021.103685
Reference: MRC 103685

To appear in: *Mechanics Research Communications*

Received date: 10 February 2021
Revised date: 22 February 2021
Accepted date: 23 February 2021

Please cite this article as: Sai Sharan Injeti, Nihit Vyas, Ratna Kumar Annabattula, Modified Stoney's equation with anisotropic substrates undergoing large deformations, *Mechanics Research Communications* (2021), doi: https://doi.org/10.1016/j.mechrescom.2021.103685

Highlights

- Mismatch strain-curvature relations for thin films on anisotropic substrate under large deformation.
- Comparison of the analytical results with numerical simulations for Silicon wafer substrates.
- The derived expressions for anisotropic substrates show improvement over existing results in the literature.

Modified Stoney's equation with anisotropic substrates undergoing large deformations

Sai Sharan Injeti[a], Nihit Vyas[b], Ratna Kumar Annabattula[b,*]

[a]*Division of Engineering and Applied Science, California Institute of Technology, Pasadena, CA 91125, USA*
[b]*Department of Mechanical Engineering, Indian Institute of Technology Madras, Chennai 600036, India*

Abstract

Thin film deposition is a key fabrication step in several opto-mechanical and electronics applications. For instance, thin film coatings can act as reflective interfaces, protective coatings or they can be used to modify the thermal behavior of the film-substrate system. For effective design, it is important to understand the deformation of the system in response to residual stresses during thin film deposition. The widely used Stoney's equation to measure this deformation assumes isotropic elasticity of the substrate together with infinitesimal strains and rotations. In this work we relax both constraints, where we study the deformation of commonly used substrates made of single crystal Si(001) and Si(111) wafers that undergo large rotations. We derive relations between normalized substrate curvature and thin film mismatch strain and validate our analysis with numerical results. The methodology presented can be used for more accurate understanding of a broad range of film-substrate systems in semiconductors.

Keywords: Stoney's equation, thin film, anisotropic substrate, large deformation

1. Introduction

The thin film - substrate configuration assumes a curvature due to a mismatch strain (e.g., elastic, thermal) between the film and the substrate. The curvature of such systems are commonly expressed in terms of the residual stress present in the film through the Stoney equation [1], given by

$$\sigma_f = \frac{E_s h_s^2}{6(1-\nu_s)h_f}\kappa, \tag{1}$$

where σ_f is the equi-biaxial residual stress in the film, κ is the uniform spherical curvature of the film-substrate configuration, h_f is the film thickness and h_s is the thickness of the substrate. Eq. 1 assumes the substrate material to be elastically isotropic with E_s being its modulus of elasticity and ν_s being the Poisson's ratio. Along with the isotropic substrate assumption, there are several other assumptions [2; 3] made while deriving Eq. (1), including small rotations in deformation. Assumptions that the rotations are infinitesimally small and that the substrate material is elastically isotropic are relaxed in this paper. Modifications to the original Stoney equation have been gaining importance since its first appearance. This is evident from papers published in recent years addressing or enhancing its accuracy using improved methods [4; 5] to extending it to a non-uniform stress state [6]. Modified curvature relations were proposed by Nix [7], which use Silicon wafer substrates. Later, the modified Stoney equation considering thin and elastically isotropic substrates was derived by Freund et al. [2]. The equation that relates the substrate curvature to the thin film mismatch in the non-linear deformation range for elastically isotropic and thick substrates is given by Freund [3]

$$S = K[1 + (1-\nu_s)K^2], \tag{2}$$

where $S = [3\epsilon_m R^2 h_f E_f(1-\nu_s)]/[2h_s^3 E_s(1-\nu_f)]$ is the normalized mismatch strain in the film, and $K = R^2\kappa/(4h_s)$, is the normalized curvature. The stress-curvature relations for thick and anisotropic substrates in the small deformation regime were derived by Janssen, Abdalla, van Keulen, Pujada, and van Venrooy [8]. The stress-curvature

*Corresponding author, Tel: +91-44-2257-4719
Email addresses: `sinjeti@caltech.edu` (Sai Sharan Injeti), `ratna@iitm.ac.in` (Ratna Kumar Annabattula)

relation for Si(001) and Si(111) wafers are given by

$$\sigma_f h_f = \frac{h_s^2}{6(s_{11}^{Si} + s_{12}^{Si})R}, \tag{3}$$

$$\sigma_f h_f = \left(\frac{6}{4s_{11}^{Si} + 8s_{12}^{Si} + s_{44}^{Si}}\right)\frac{h_s^2}{6R}, \tag{4}$$

respectively, where s_{ij}^{Si} are elements of the compliance matrix of Si substrate. The anisotropy in material properties may lead to anisotropy in the stress state [9]. But the discussion in this paper is restricted to a system in which the film is under the influence of an equibiaxial stress.

1.1. Scope of the paper

In this paper, Eq. (2) is extended to configurations with single crystal Si(001) and Si(111) wafer substrates. These equations are derived by minimizing the potential energy of the system considering small strains but large rotations along with linear elastic anisotropy of the substrate. A similar analysis was used by Injeti and Annabattula [10] to derive the Stoney equation for systems with thin and anisotropic substrates in the small deformation regime. Numerical results for curvatures of Si wafer substrates in the non-linear deformation range are presented. Deviations of curvatures obtained from the derived equations and equations (3) and (4) from the numerical results are discussed, in a broad range of thin film mismatch strain.

2. Mathematical Formulation and Derivation

In this section, a circular film-substrate system is analyzed with the assumption of uniform curvature for simple analytical treatment. However, it is to be noted that the curvature of the system in the non-linear deformation regime varies across the plane of the substrate [11]. This variation is captured by the numerical results presented in the next section and is compared with the derived result. Figure 1 shows the cross sectional view of the thin film-substrate system, where h_s, h_f and R represent the thickness of the substrate, thickness of the film and radius of the circular system, respectively. Deformation in the configuration is measured using a cylindrical coordinate system (r, θ, z). The origin of the coordinate system is considered to be at the intersection of the substrate mid-plane and the axis of symmetry of the system. For thin films ($h_f << h_s$), the stress in the film across its thickness varies negligibly and the force acting on the substrate in Stoney's equation (left hand side in equations (1), (3) and (4)) is calculated as the force on the substrate per unit width. For the case when the film is thick, this forcing term needs to be modified as the integral of stress in the film over h_f [12]. In this work, we consider thin films, with a uniform distribution of stress across its thickness causing a radially symmetric deformation in the system. The radial stress (σ_{rr}) and the circumferential stress ($\sigma_{\theta\theta}$) are the only non zero components of stress in the substrate and film because the deformation is axially symmetric and the out-of-plane stress (σ_{zz}) is assumed to be negligible. Hence, the elastic strain energy density in the film and substrate materials can be represented as

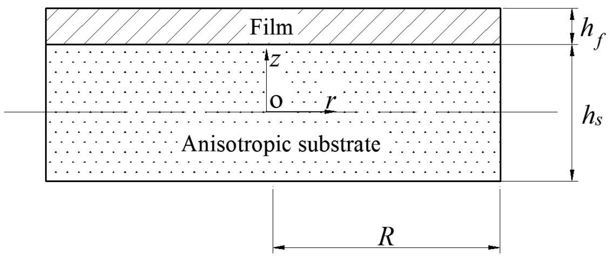


Figure 1: Schematic showing the cross section of a circular thin film deposited on an anisotropic substrate

$$U(r,z) = \frac{1}{2}(\sigma_{rr}\epsilon_{rr} + \sigma_{\theta\theta}\epsilon_{\theta\theta}), \tag{5}$$

where, ϵ_{rr} and $\epsilon_{\theta\theta}$ are the radial and circumferential strain components, respectively. Let the radial and transverse displacements at a point on the substrate mid-plane be represented by $u(r)$ and $w(r)$, respectively. Then, ϵ_{rr} and $\epsilon_{\theta\theta}$ for large deformations can be written as [2]

$$\epsilon_{rr}(r,z) = u'(r) - zw''(r) + \frac{1}{2}w'(r)^2 + \epsilon_m,$$
$$\epsilon_{\theta\theta}(r,z) = \frac{u(r)}{r} - \frac{zw'(r)}{r} + \epsilon_m. \tag{6}$$

In Eq. (6), the derivatives are considered with respect to the radial coordinate, r. The term $\frac{1}{2}w'(r)^2$ in ϵ_{rr} is the contribution to the extensional strain at the mid-plane due to the transverse deformation. This term is neglected in the original Stoney equation (Eq. (1)), as the rotations are assumed to be small. However, a flat plane deforming into a spherical surface must be accompanied with a stretch or compression of the substrate mid plane. Hence, including the higher order term in the extensional strain considers finite rotations, but still under small strain, which implies the material model of a linear elastic anisotropic substrate used in the following section remains valid. The misfit strain in the system, ϵ_m, is assumed to be accommodated in the film alone [2].

2.1. *Curvature-mismatch relation for thin Si(001) wafer substrate*

In the Si(001) wafer, the plane of the wafer is perpendicular to the [001] direction, which is along the z-axis of the deformation coordinate system. The r and θ directions of the deformation coordinate axes are represented by two orthogonal directions in the plane of the single crystal wafer. Hence, the crystallographic axes of the Si(001) wafer also coincide with the axes of deformation. The stress and strain tensors are related through the elastic stiffness or compliance matrix as [8]

$$\begin{pmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{pmatrix} = \begin{pmatrix} c_{11} & c_{12} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{11} & c_{12} & 0 & 0 & 0\\ c_{12} & c_{12} & c_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & c_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & c_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & c_{44}\end{pmatrix}\begin{pmatrix}\epsilon_{11}\\ \epsilon_{22}\\ \epsilon_{33}\\ 2\epsilon_{23}\\ 2\epsilon_{13}\\ 2\epsilon_{12}\end{pmatrix},$$

$$\begin{pmatrix}\epsilon_{11}\\ \epsilon_{22}\\ \epsilon_{33}\\ 2\epsilon_{23}\\ 2\epsilon_{13}\\ 2\epsilon_{12}\end{pmatrix} = \begin{pmatrix} s_{11} & s_{12} & s_{12} & 0 & 0 & 0\\ s_{12} & s_{11} & s_{12} & 0 & 0 & 0\\ s_{12} & s_{12} & s_{11} & 0 & 0 & 0\\ 0 & 0 & 0 & s_{44} & 0 & 0\\ 0 & 0 & 0 & 0 & s_{44} & 0\\ 0 & 0 & 0 & 0 & 0 & s_{44}\end{pmatrix}\begin{pmatrix}\sigma_{11}\\ \sigma_{22}\\ \sigma_{33}\\ \sigma_{23}\\ \sigma_{13}\\ \sigma_{12}\end{pmatrix}. \tag{7}$$

Here σ_{ij} and ϵ_{ij} are the components of stress and strain tensors, respectively, where i and j take values 1,2 or 3. In the calculations to follow, we replace 1 by r, 2 by θ and 3 by z in stress and strain notations to remain consistent with the polar coordinate system chosen. c_{11}, c_{12} and c_{44} are elastic stiffness constants and s_{11}, s_{12} and s_{44} are the elastic compliance constants. In the substrate material, from Eq. (7)

$$\begin{aligned}\sigma_{rr} &= \left(\frac{c_{11}^2-c_{12}^2}{c_{11}}\right)\epsilon_{rr} + \left(\frac{c_{11}c_{12}-c_{12}^2}{c_{11}}\right)\epsilon_{\theta\theta},\\ \sigma_{\theta\theta} &= \left(\frac{c_{11}c_{12}-c_{12}^2}{c_{11}}\right)\epsilon_{rr} + \left(\frac{c_{11}^2-c_{12}^2}{c_{11}}\right)\epsilon_{\theta\theta}.\end{aligned} \tag{8}$$

In order to preserve the uniform curvature (κ) assumption, the parametric forms for the substrate mid-plane deflections are adopted as $u(r) = \epsilon_0 r + \epsilon_1 r^3$, $w(r) = \kappa r^2/2$ [2]. From Eq. (6)

$$\begin{aligned}\epsilon_{\theta\theta} &= \epsilon_0 + \epsilon_1 r^2 - \kappa z + \epsilon_m,\\ \epsilon_{rr} &= \epsilon_{\theta\theta} + r^2\left[2\epsilon_1 + \frac{\kappa^2}{2}\right] = \epsilon_{\theta\theta} + r^2\alpha.\end{aligned} \tag{9}$$

From equations (5), (8) and (9) the elastic strain energy density in the substrate material can be written as

$$U^s(r,z) = \frac{c_{11}^2 + c_{11}c_{12} - 2c_{12}^2}{c_{11}}\left(\epsilon_{\theta\theta}^2 + \epsilon_{\theta\theta}r^2\alpha\right) + \frac{c_{11}^2-c_{12}^2}{c_{11}}\left(\frac{r^4\alpha^2}{2}\right). \tag{10}$$

For the elastically isotropic film, let ν_f and E_f denote the Poisson's ratio and the Young's modulus of elasticity, respectively. Using equations (5) and (9), the strain energy density in the film for plane stress can be written as

$$U^f(r,z) = M_f\left(\epsilon_{\theta\theta}^2 + \epsilon_{\theta\theta}r^2\alpha\right) + \frac{M_f}{1+\nu_f}\left(\frac{r^4\alpha^2}{2}\right). \tag{11}$$

Here, $M_f = E_f/(1-\nu_f)$ represents the biaxial modulus of the film material. We can rewrite Eq. (10) as

$$U^s(r,z) = M_s\left(\epsilon_{\theta\theta}^2 + \epsilon_{\theta\theta}r^2\alpha\right) + \frac{c_{11}^2-c_{12}^2}{c_{11}}\left(\frac{r^4\alpha^2}{2}\right). \tag{12}$$

where $M_s = (c_{11}^2 + c_{11}c_{12} - 2c_{12}^2)/c_{11}$ represents an equivalent biaxial modulus for the Si(001) [8; 10; 13]. The potential energy of the substrate and film can be written as

$$\begin{aligned}V^s(\epsilon_0,\epsilon_1,\kappa) =& 2\pi\int_0^R\int_{-h_s/2}^{h_s/2}\left[M_s\left(\epsilon_{\theta\theta}^2+\epsilon_{\theta\theta}r^2\alpha\right)\right.\\ &\left.+\frac{c_{11}^2-c_{12}^2}{c_{11}}\left(\frac{r^4\alpha^2}{2}\right)\right]rdrdz,\end{aligned} \tag{13}$$

$$\begin{aligned}V^f(\epsilon_0,\epsilon_1,\kappa) =& 2\pi\int_0^R\int_{h_s/2}^{h_f+h_s/2}\left[M_f\left(\epsilon_{\theta\theta}^2+\epsilon_{\theta\theta}r^2\alpha\right)\right.\\ &\left.+\frac{M_f}{1+\nu_f}\left(\frac{r^4\alpha^2}{2}\right)\right]rdrdz,\end{aligned} \tag{14}$$

respectively. For the equilibrium condition of stationary potential energy to hold, $\partial V/\partial\kappa$, $\partial V/\partial\epsilon_0$ and $\partial V/\partial\epsilon_1$ must be equal to 0, where $V = V_s + V_f$ is the total potential energy of the system. Solving $\partial V/\partial\epsilon_0 = 0$ and $\partial V/\partial\epsilon_1 = 0$ for ϵ_0 and ϵ_1 in terms of κ, and substituting them back in $\partial V/\partial\kappa = 0$ gives the desired expression for the curvature. These equations have been simplified for an analogous case when the substrate material is isotropic and $h_f/h_s \ll 1$, by Freund [3]. Extending the same approach to the case when the substrate material is made from Si(001) wafer, the condition for stationary potential energy results in

$$S = K\left[1 + \left(\frac{c_{11}}{c_{11}+c_{12}}\right)K^2\right], \tag{15}$$

where, $S = 3\epsilon_m R^2 h_f M_f/(2h_s^3 Ms)$ and $K = R^2\kappa/(4h_s)$ are the normalized mismatch strain and normalized curvature, respectively.

2.2. Curvature-mismatch relation for thin Si(111) wafer substrate

In the Si(111) wafer, the plane of the wafer is perpendicular to the [111] direction. The constitutive equation is written in the frame of the Si crystal while the deformation of the substrate takes place in the frame of the wafer, which in this case does not match. The reference frame of the constitutive equation in Si(111) wafer has been transformed to align with the coordinate system describing the deformation of the substrate. We describe this transformation similar to the one outlined by Injeti and Annabattula [10].

Let $\boldsymbol{x_1} = (1\,0\,0)^T$, $\boldsymbol{x_2} = (0\,1\,0)^T$ and $\boldsymbol{x_3} = (0\,0\,1)^T$ be the orthonormal basis that describes the frame of the Si crystal. Let $\tilde{\boldsymbol{x}}_1 = \frac{1}{\sqrt{2}}(1\,-1\,0)^T$, $\tilde{\boldsymbol{x}}_2 = \frac{1}{\sqrt{6}}(1\,1\,-2)^T$ and $\tilde{\boldsymbol{x}}_3 = \frac{1}{\sqrt{3}}(1\,1\,1)^T$ be the orthonormal basis that describes the frame of the wafer. Note that $\tilde{\boldsymbol{x}}_3$ is perpendicular to the plane of the wafer, and $\tilde{\boldsymbol{x}}_1$ and $\tilde{\boldsymbol{x}}_2$ are two orthogonal directions in the plane of the wafer. Note that $\tilde{\boldsymbol{x}}_1$ and $\tilde{\boldsymbol{x}}_2$ can be arbitrary mutually orthonormal in-plane vectors. Let the rotation matrix to align the basis $(\boldsymbol{x_1}, \boldsymbol{x_2}, \boldsymbol{x_3})$ with $(\tilde{\boldsymbol{x}}_1, \tilde{\boldsymbol{x}}_2, \tilde{\boldsymbol{x}}_3)$ be given by $\boldsymbol{T}$. It is straightforward to calculate that

$$\boldsymbol{T} = \begin{pmatrix} \frac{1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ \frac{-1}{\sqrt{2}} & \frac{1}{\sqrt{6}} & \frac{1}{\sqrt{3}} \\ 0 & \frac{-2}{\sqrt{6}} & \frac{1}{\sqrt{3}} \end{pmatrix}$$

Owing to the orthogonality of the rotation matrix, the components of transformed stress and strain tensors can be calculated as $\tilde{\sigma}_{ij} = T_{ip}T_{jq}\sigma_{pq}$ and $\tilde{\epsilon}_{ij} = T_{ip}T_{jq}\epsilon_{pq}$, respectively [14]. Here each index can take values from 1 to 3, and summation is implied over repeated indices. As indicated in section 2.1, indices 1, 2, 3 represent r, θ and z, respectively. It is straightforward to calculate the transformed elastic compliance elements that relate the transformed stress and strain, from Eq. (7) and outlined by Injeti and Annabattula [10]. Then the radial and circumferential strains can be written as

$$\tilde{\epsilon}_{rr} = \left(\frac{s_{11}}{2} + \frac{s_{12}}{2} + \frac{s_{44}}{4}\right)\tilde{\sigma}_{rr} + \left(\frac{s_{11}}{6} + \frac{5s_{12}}{6} - \frac{s_{44}}{12}\right)\tilde{\sigma}_{\theta\theta},$$
$$\tilde{\epsilon}_{\theta\theta} = \left(\frac{s_{11}}{6} + \frac{5s_{12}}{6} - \frac{s_{44}}{12}\right)\tilde{\sigma}_{rr} + \left(\frac{s_{11}}{2} + \frac{s_{12}}{2} + \frac{s_{44}}{4}\right)\tilde{\sigma}_{\theta\theta}. \tag{16}$$

Let $A = \frac{s_{11}}{2} + \frac{s_{12}}{2} + \frac{s_{44}}{4}$ and $B = \frac{s_{11}}{6} + \frac{5s_{12}}{6} - \frac{s_{44}}{12}$. It follows that $\tilde{\sigma}_{rr} = \frac{1}{A^2-B^2}(A\tilde{\epsilon}_{rr} - B\tilde{\epsilon}_{\theta\theta})$ and $\tilde{\sigma}_{\theta\theta} = \frac{1}{A^2-B^2}(A\tilde{\epsilon}_{\theta\theta} - B\tilde{\epsilon}_{rr})$. From equations (5) and (9)

$$U^s(r,z) = M'_s\left(\tilde{\epsilon}^2_{\theta\theta} + \tilde{\epsilon}_{\theta\theta}r^2\alpha\right) + \frac{A}{A^2-B^2}\left(\frac{r^4\alpha^2}{2}\right), \tag{17}$$

where $M'_s = 6/(4s_{11} + 8s_{12} + s_{44})$ represents the equivalent biaxial modulus of the Si(111) wafer material. Following the similar approach as with Si(001) wafer substrate, the curvature-mismatch relation for this case results in

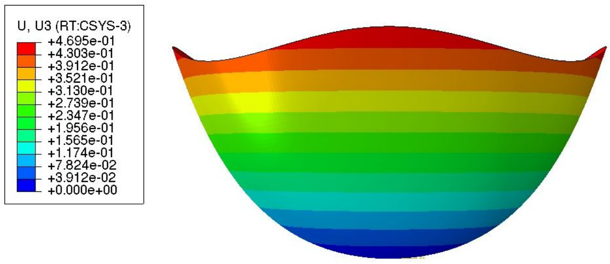
$$S = K\left[1 + \frac{4}{3}\left(\frac{2s_{11} + 4s_{12} + \frac{1}{2}s_{44}}{2s_{11} + 2s_{12} + s_{44}}\right)K^2\right]. \tag{18}$$

For an anisotropic film, an appropriate biaxial modulus may be used in the place of M_f to calculate the normalized mismatch strain S.

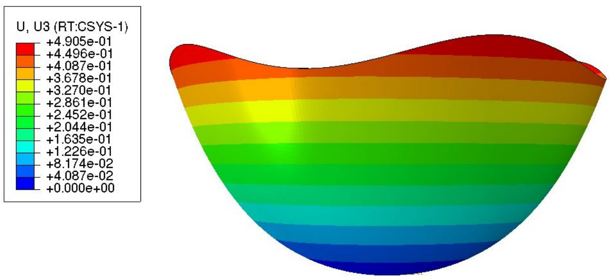
3. Numerical Results and Discussion

The deformations are studied with simulations performed using commercial finite element software Abaqus [15]. The thin-film configuration is modeled using four-noded composite shell elements. This choice allows a distribution in material properties across the thickness of the shell. The geometric non-linearities due to large rotations are also accounted for in the simulation. In Fig. 1, the parameters h_s/h_f and R/h_s are fixed at 20 and 50, respectively. Following this, the undeformed radius of the system is chosen to be 10 mm. The mismatch strain is provided to the system in the form of thermal strain. For the ease of numerical simulation, the film and substrate materials in both cases have been chosen to have identical mechanical properties, but varying thermal expansion coefficients. In Fig. 2, the thermal expansion coefficient of the bottom layer is taken to be 10^{-5}/ °C and that of the top layer is set at 0/ °C, while both layers are subjected to the same temperature rise to produce the appropriate mismatch strain (note that the mismatch strain ultimately depends on the difference and not the individual thermal expansion coefficients of each layer). Also, the ratio of biaxial moduli (M_f/M_s) is one in both simulations. The stiffness constants of silicon obtained by McSkimin and Jr. [16] are used in order to simplify equations (15) and (18). The biaxial moduli used for the substrates Si(001) and Si(111), i.e. M_s in the simulation are 1.803×10^{-11} Nm^{-2} and 2.291×10^{-11} Nm^{-2}, respectively [8].

The transverse deflections for the Si(001) substrate along $\boldsymbol{d}_1^{(001)} = [1\,\bar{1}\,0]$, $\boldsymbol{d}_2^{(001)} = [1\,1\,0]$, $\boldsymbol{d}_3^{(001)} = [\bar{1}\,1\,0]$ and $\boldsymbol{d}_4^{(001)} = [\bar{1}\,\bar{1}\,0]$ directions are computed for varying normalized mismatch strains. A similar approach was



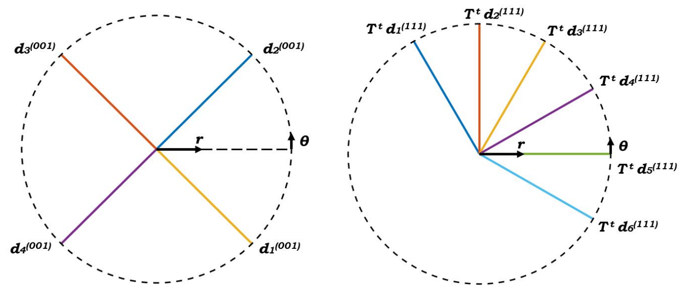
(a)



(b)

Figure 2: The simulation result showing deflection along z-axis induced in (a) Si(001) substrate and (b) Si(111) substrate, in mm subject to the same temperature rise.

used by Janssen et al. [8] in order to determine the average curvature of anisotropic substrates for small deformations, experimentally. The directions are described in the frame of the wafer, which is the same as the frame of the Si crystal. The directions are indicated by the solid colored lines in Fig. 3(a). The dashed curve represents the circular substrate. The radial curvature along each direction, $k(r)$ is calculated by first fitting an eighth order polynomial in r, $w(r)$ to the deflection data and then determining the curvature as $w''(r)/(w'(r)^2+1)^{3/2}$. The normalized curvature along each direction as a function of r is calculated as $K(r) = R^2 k(r)/4h_s$. The function value at each radial position is then averaged over the four directions. A similar approach is followed to calculate the average normalized curvature as a function of r for the Si(111) substrate configuration. Here, the deflections along the z-axis are measured along the $\boldsymbol{d}_1^{(111)} = [0\ 1\ \bar{1}]$, $\boldsymbol{d}_2^{(111)} = [1\ 1\ \bar{2}]$, $\boldsymbol{d}_3^{(111)} = [1\ 0\ \bar{1}]$, $\boldsymbol{d}_4^{(111)} = [2\ \bar{1}\ \bar{1}]$, $\boldsymbol{d}_5^{(111)} = [1\ \bar{1}\ 0]$ and $\boldsymbol{d}_6^{(111)} = [1\ \bar{2}\ 1]$ directions, each separated by an angle of 30 degrees. Note that these directions are described in the frame of the wafer, which is different from the frame of the Si crystal. The colored solid lines in Fig. 3(b) indicate these directions in the frame of the Si crystal using the transformation described in section 2.2. We consider directions in Si(111) that do not span the entire circular cross-section, as the deformation is symmetric for reflections about planes with normals along the cricular cross-section.



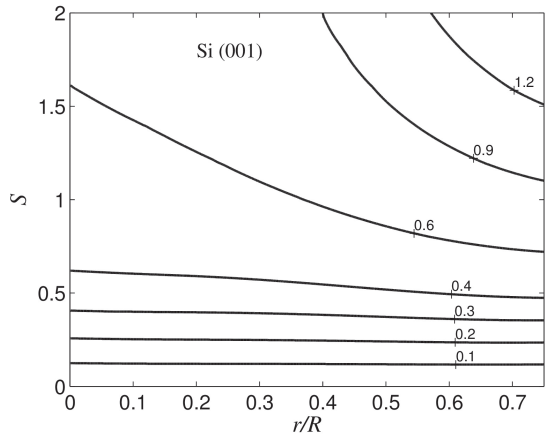
(a) (b)

Figure 3: Directions along which the deformation is measured for (a) Si(001) and (b) Si(111) substrate.

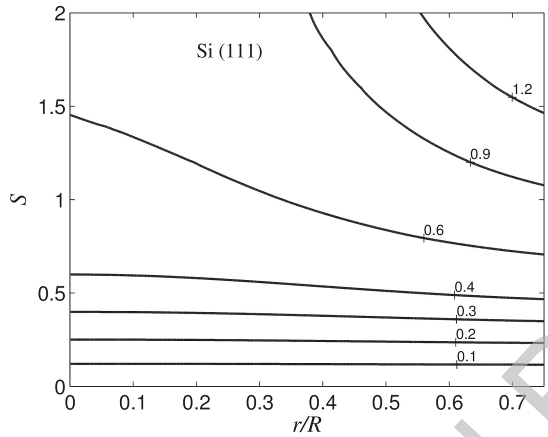
Fig. 4 shows the plots between normalized mismatch strain (S) and normalized distance (r/R) for different normalized curvature (K) values, obtained from numerical simulations. The figure indicates uniform curvature across the substrate mid plane for smaller values of S, for both Si(001) and Si(111) substrates. As the mismatch strain is increased, the curvature is increasingly non-linear. Hence, the uniform curvature assumption is reasonable for normalized mismatch strains that are less than 0.3. A similar observation was made by Freund [3] for thin film configurations with isotropic substrates undergoing large deformations. On substituting isotropic material properties for the substrate in the numerical simulation, the results obtained by Freund [3] have been reproduced (results not shown here). Furthermore, the non-uniform curvature occurs at a smaller mismatch for anisotropic substrates when compared to the isotropic substrate used in Freund's work [3]. This observation is possibly due to the direction dependence of curvature in anisotropic substrates.

Fig. 5 shows the plots between normalized curvature (K) and normalized mismatch strain (S) for different r/R values. Also the curvature obtained from the present large deformation analysis (solid line) is compared with small deformation (dotted line) and finite element results (dashed lines). The figure indicates that the curvatures obtained from equations (15) and (18) (i.e., large deformation equations) lie within the curvature values obtained from the finite element simulations. Whereas, equations (3) and (4) (i.e., small deformation equations) overestimate the curvature.

In Fig. 6, k_{15} and k_{18} correspond to curvatures obtained from equations (15) and (18), respectively. k_3 and k_4 are curvatures obtained from equations (3) and (4), re-

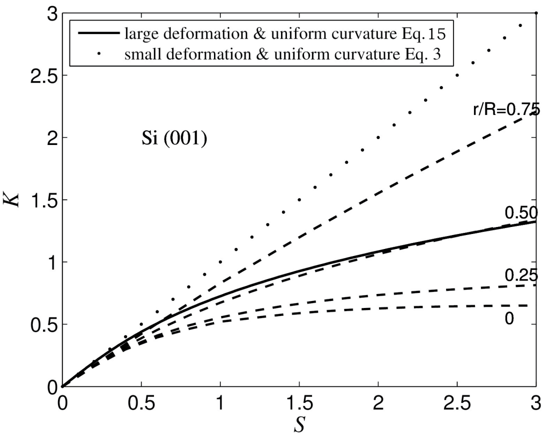


(a)

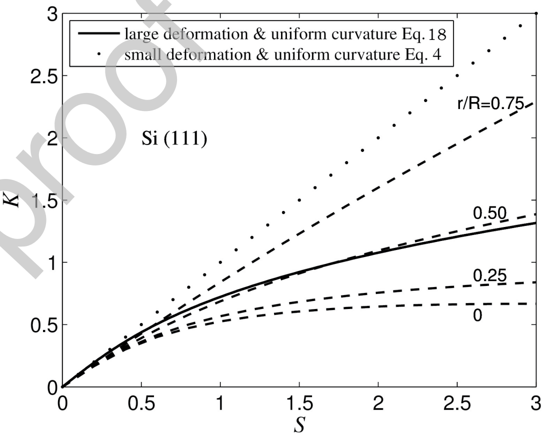


(b)

Figure 4: Contour plots of normalized curvature K as the normalized mismatch strain S and normalized distance r/R are varied for the system with (a) Si(001) substrate and (b) Si(111) substrate.



(a)



(b)

Figure 5: Plot for normalized curvature $K(r)$ vs mismatch strain S for small and large deformations for systems with (a) Si(001) and (b) Si(111) substrates. The dashed lines plot finite element simulations at four values of r/R.

spectively. In figures 6(a) and 6(b), k_{FEA} is the curvature estimated from the finite element simulations for Si(001) and Si(111) wafer substrates, respectively. k_{FEA} is calculated by taking the average of curvatures for a given mismatch strain, over the four equally spaced radii starting from the substrate centre. It can be observed that the deviations are much larger for curvatures obtained from equations (3) and (4) when compared to equations (15) and (18), indicating that the derived formulae are a better fit to the data obtained from the finite element simulations, as they account for large deformations in the configuration. Furthermore, a semi-analytical model for the curvature (at r=0) of Si-doped GaN on Si (111) substrate undergoing large deformations, was presented by Clos, Dadgar, and Krost [17]. The deviation of this central curvature with respect to the curvature obtained from Eq. (18) is about 32% for a thickness ratio (h_f/h_s) of 0.01. Whereas, this deviation is as high as 83% for the same thickness ratio, when the curvature is calculated from the small deformation Stoney formula (Eq. (4)). This further supports the use of eq. (18) over eq. (4) for Si (111) substrates deforming in the non-linear regime.

4. Conclusions

In summary, normalized curvature-mismatch relations are derived for thin films bonded to anisotropic substrates (Equations (15) and (18)) undergoing large deformations.

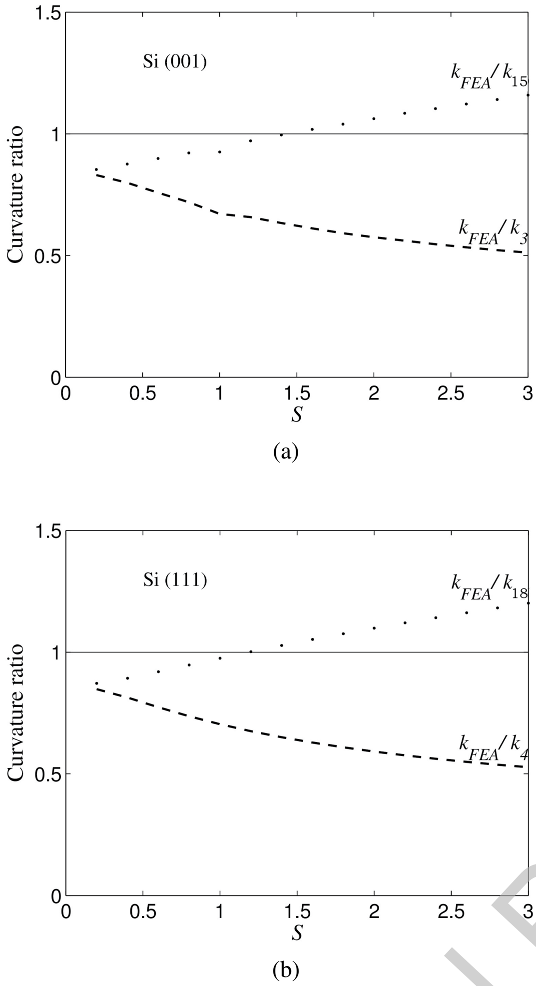


Figure 6: Deviation of the curvatures obtained from (a) equations (15) and (3), and (b) equations (18) and (4), from the finite element simulation.

The potential energy containing a contribution from extensional strain due to finite rotations is considered. Equations (15) and (18) can be extended to elastically anisotropic films by calculating an appropriate biaxial modulus for M_f, depending on the material. The formulae derived for large deformations along with existing expressions for small deformations for anisotropic substrates are compared with numerical results obtained using Abaqus FEA. Furthermore, the curvature obtained from the numerical data is almost uniform across the radius of the substrate for normalized mismatch (S) values within 0.3, for both Si(001) and Si(111) substrates. The direction dependence of curvature in anisotropic substrates is evident from the observation that non-uniformity in substrate curvature occurs at a smaller mismatch strain when compared to isotropic substrates. The analytical formulae derived for large deformations (Equations (15) and (18)) match the finite element results better, when compared to the formulae derived using small deformation assumption.

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